CAMS Planning Workshop

Purpose and objectives

Wednesday April 4, 2006

Idaho National Laboratory

The CAMS Mission

Ensure that the Idaho National has the computing resources (human, hardware, software, communications and collaborations) needed to support its goal of becoming the preeminent national nuclear energy laboratory with synergetic world-class multi-program capabilities.

FY06: Initiate CAMS and lay foundation

Objectives of Workshop

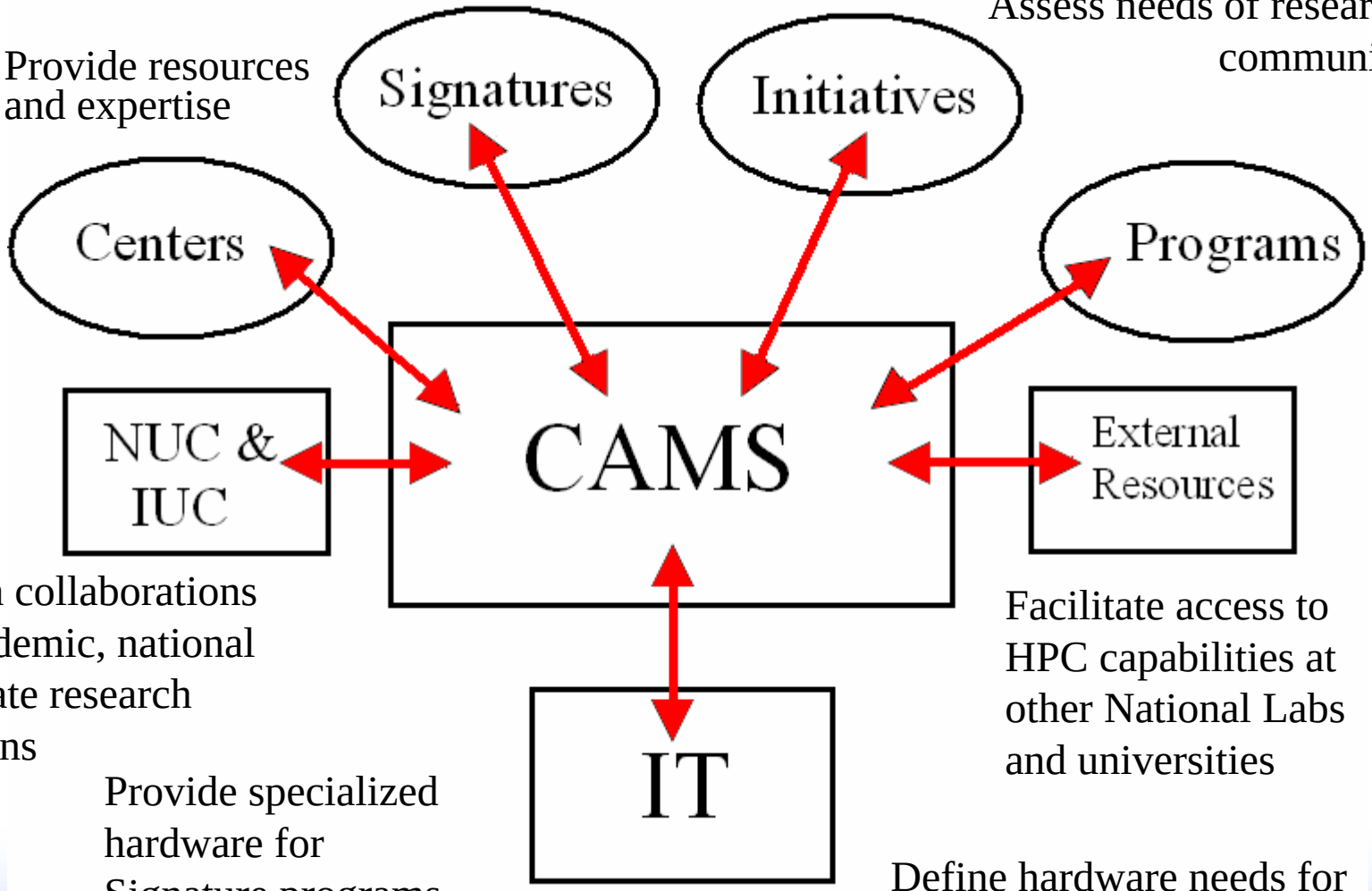
- Reassess INL research and computing priorities and needs
- Revise CAMS Roadmap to reflect new realities and priorities

INL Computational Environment

Develop and maintain software suite

Assess needs of research community

Provide resources and expertise



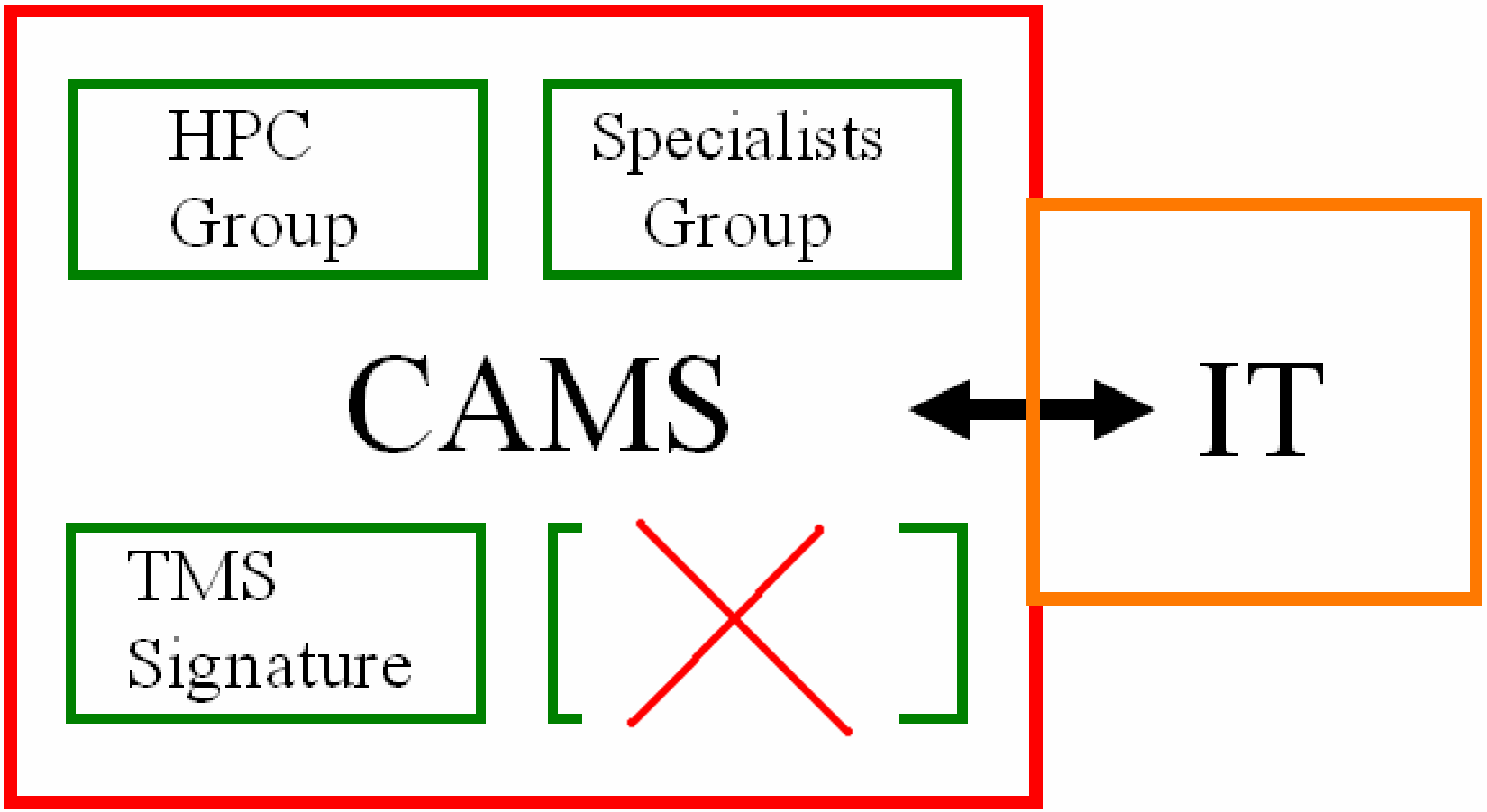
Establish collaborations with academic, national and private research institutions

Facilitate access to HPC capabilities at other National Labs and universities

Provide specialized hardware for Signature programs

Define hardware needs for INL research community & communicate needs to DOE

CAMS Structure



New reality: The Computational Science Initiative will not happen in FY 2007

CAMS: Initial computational themes to support Nuclear Programs with secondary benefit to National and Homeland Security and Science and Technology

- Three-dimensional transport modeling (fluid flow, neutron transport, heat transport ….
- Materials behavior (solid and fluid materials under extreme conditions
- Instrumentation and controls (design and simulation of instrumentation and and control systems)

CAMS experts group

Science Domain Experts:

- Computational materials science
- Computational actinide chemistry
- Computational fluid dynamics

} Aligned with computational themes

Computational specialists

- Code developers
- Scientific visualization
- Hardware specialists

} Work closely with domain experts
Enhance computing capabilities and infrastructure

We need to make a transition from code users to users and developers

Computational Chemistry (actinide chemistry, materials chemistry, corrosion)

- Separation is critical to closing the nuclear fuel cycle
- Corrosion is a major problem in existing and future nuclear power plants
- The interaction between fuels and fission products has an important impact on fuels performance
- The production of hydrogen via thermochemical cycles or high temperature electrolysis entails chemical reactions that degrade catalysts and materials and threaten commercial success.
- Chemistry cuts across INL research activities: national and homeland security, subsurface science, combustion, hydrogen production and utilization

Relationships between CAMS themes and INL signatures

Science Signatures	CAMS Computational Themes				Computing Infrastructure
	3-D Transport Modeling	Materials Behavior	Controls and Instrumentation	Computational Chemistry	
Materials and Nuclear Fuels Science and Technology	X	X		X	X
Microbiological and Geological Systems	X		X	X	X
Separations and Actinide Science	X	X		X	X
Theory, Modeling, and Simulation	X	X	X	X	X
Instrumentation and Controls		X	X		X

Recommendations from CAMS Board

- Focus on one area
- Team with expertise wherever it resides (focus on young people at universities)
- Run workshops, summer schools
- Recruit young people

Possible focus areas:

- Materials in harsh environments
- Computational engineering science
- Computational actinide chemistry

High Performance Computing: New paradigms and a new challenges

- Most applications run poorly on high end computers and many research domains are not making effective use of high performance computing

- The individual investigator or small team approach no longer works – large teams that include applied mathematicians, computer scientists and research domain experts are required to develop code that runs well on high-end computers

- In many cases the required expertise does not exist in a single institution – this requires interdisciplinary inter-institutional collaborations, which have a large inherent overhead

- For the most part, INL is not well prepared or well positioned to play a leading role in the development of code that will run well on high-end computers to support its critical missions

INL will need a rapid growth in high-performance computing hardware – also a challenge

Projected high-performance computing hardware needs (processor years per year) based on 2006 survey.

FY	2007	2008	2009	2010	2011
2006 Survey	5000 (15 Tf)	9000 (27 Tf)	17000 (50 Tf)	30000 (90 Tf)	37500 (110 TF)

To reach 10% of leading National Laboratory in 10 years

2005/ 2006	2007	2008	2009	2010	2011
2 Tf ≈ 1%	5 Tf	13 Tf	35 Tf	90 Tf	330 Tf ≈3.3%

Idaho National Laboratory

A large increase in computing hardware resources will be needed to support INL programs and achieve strategic goals

FY2006 CAMS PEMP Milestones

- Establish CAMS Advisory Board by December 31, 2006: Done – met yesterday.
- Deliver HPC requirements document to DOE by June 30, 2006. The survey is complete and a draft has been prepared
- Brief DOE Office of Science, DOE Office of Nuclear Energy and NSF by July 31: Area of concern
- Analyze INL software suite, project needs and make recommendations by July 31: nearing completion (Patrick O'Leary)
- Establish computational actinide chemistry program by September 30. LDRD program (Mike Benson, PI), postdoc. hired, 2 Strategic Hire candidates will be interviewed in April, working with Chemistry Group

FY2006 CAMS PEMP Milestones (continued)

• Establish web site by June 30: Web site is almost finished (need to set up ‘public’ and ‘private’ parts and make accessible from outside) http://cams.inel.gov/ (internal) http://www.inl.gov/scienceandtechnology/cams/workshop (external for SLC workshop)

Other Milestones

• Complete plans for INL Scientific Computation Initiative by March 31: Was underway – Now halted

• Survey currently available open source software: Needs more emphasis

• Obtain access to ASCI visualization tools: Not started yet

Other FY 2006 milestones (continued)

- Organize workshops for access to leadership class computing facilities: First workshop held in SLC on March 23 and 24

- Establish web site by June 30: Web site is almost finished (need to set up ‘public’ and ‘private’ parts and make accessible from outside)

- Establish CAMS modeling and simulation seminar series by Dec 31, 2005 and initiate seminars by March 3, 2006: Done well ahead of time – seven seminars so far.

FY2006 CAMS PEMP Milestones (continued)

- Establish web site by June 30: Web site is almost finished (need to set up ‘public’ and ‘private’ parts and make accessible from outside)

Other Milestones

- Interface with State of Idaho and Idaho business: Presentations to visiting groups
- Survey currently available open source software: Needs more emphasis
- Obtain access to ASCI visualization tools: Not started yet
- Organize workshops for access to leadership class computing facilities: First workshop held in SLC on March 23 and 24

Other Accomplishments

- Organized and supported preparation of two SciDAC proposals
- CAMS is working with IT to ensure that INL scientists and engineers play key decision making roles in all aspects of scientific, engineering and high performance computing.
- Working groups established: Hardware selection, HPC priorities, Internal CAMS Advisory Board, Software quality, Computational Science Initiative, Tailored systems for distinctive signatures, software needs and licensing.

Theory Modeling and Simulation (TMS) Distinctive Signature

The distinctive signatures will serve to attract preeminent scientific researchers, foster new program opportunities, engender a new scientific spirit, and promote the recognition that INL offers unique scientific and engineering careers: INL Strategic Plan

TMS Distinctive Signature currently supports 7 LDRD projects: $900k - $1,000k in FY2006 ($600k in FY 2007)

Develop FY07 LDRD call to ensure that TMS project portfolio provides largest possible benefit to the INL

Theory Modeling and Simulation Distinctive Signature – LDRD Programs (reviewed on March 13)

1. Materials Damage Evolution and Failure (05-14): Clint Van Siclen)

2. Reactor Physics Methods Development for Idaho National Laboratory Competitiveness in Next Generation Nuclear Plant (NGNP) Design (05-106): Abderrafi Ougouag (PI), William K. Terry, Hans D. Gougar and Youssef Shatilla

3. Development of Integrated Virtual Engineering Tools to Facilitate Unique High-Level Decision Making Capabilities (05-098): Christopher Wright, Kevin L. Kenney , J. Richard Hess and Kenneth M. Bryden (Iowa State)

4. Modeling complexes containing actinide elements (06-057). Michael T. Benson, R. Scott Herbst and Dean R. Peterman

Theory Modeling and Simulation Distinctive Signature – LDRD Programs (provisional)

5. Computational modeling of catalysts for the reduction of sulfur trioxide in the sulfur-iodine (S-I) cycle for hydrogen production (06-039). Hellen H. Farrell (PI), Lucia Petkovic, Patrick J. Pinhero and Daniel M. Ginosar

6. Mathematical characterization and synthetic generation of spatial structures across multiple scales using fractal techniques (06-058). Charles R. Tolle (PI) and Thomas K. Larson.

7. Kinetic Monte Carlo method for calculation of diffusion coefficients for defects in solids (06-088): Clint Van Siclen

Theory Modeling and Simulation Distinctive Signature – LDRD Call

- $600k mortgage - $500k new projects
- Encourages transition from desk-top to HPC
- Encourages collaborations with high quality university faculty
- Encourages code development research
- Support and strengthen high priority INL programs